Advancement in Fuel Spray and Combustion Modeling for Compression Ignition Engine Applications

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14th May, 2013

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Project ID # ACE075

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Overview

Timeline

Project start: April 1st 2012

Partners

Project Lead: Sibendu Som
Argonne National Laboratory
Chemical Science and Engineering
Mathematics and Computing Science
Leadership Computing Facility

Convergent Science Inc. {CRADA}
Caterpillar Inc.
Cummins Engine Company {CRADA}
Chrysler LLC.

Lawrence Livermore National Laboratory
Sandia National Laboratory (Engine Combustion Network [ECN])
Advanced Engine Combustion (AEC) Working group

University of Connecticut
Politecnico di Milano, University of Perugia (Italy)

Barriers

- "Inadequate understanding of stochastics of fuel injection"
- "Improving the predictive nature of spray and combustion models"
- "Incorporating more detailed chemical kinetics into fluid dynamics simulations"
- "Development of High-Performance Computing (HPC) tools to provide unique insights into the spray and combustion processes"

Budget

FY 12: 350 K
FY 13: 500 K

Objectives

In general Engine simulations involve:

- Unresolved Nozzle flow
- Simplified combustion models
- Coarse mesh => grid-dependence
- Poor load-balancing algorithms
- Simplified turbulence models

Extensive tuning to match experimental data

High-Fidelity Approach:

- Detailed chemistry based combustion models
- Fine mesh => grid-convergence
- Improved load-balancing algorithms with METIS
- High-fidelity turbulence models: LES based
- Two-phase physics based fuel spray and nozzle-flow models

+

- High-Performance Computing

Towards Predictive Simulation of the Internal Combustion Engine

Relevance

- **Nozzle flow and Spray research**
  - Fuel spray breakup in the near nozzle region plays a central role in combustion and emission processes
  - Improving in-nozzle flow and turbulence predictions is key towards the development of predictive engine models

- **Combustion modeling using detailed chemistry**
  - Accurate chemical kinetics for fuel surrogates are key towards developing predictive combustion modeling capability
    - Mixture of n-dodecane + m-xylene is a more suitable diesel surrogate

- **High-Performance Computing**
  - Current state-of-the-art for engine simulations in OEMs involve up to 50 processors (approx.) only
  - Will be needed in order for OEMs to retain quick turn-around times for engine simulations (which may not be possible as the resolution, spray, turbulence, and chemical kinetic models become more detailed)

Milestones, FY 13

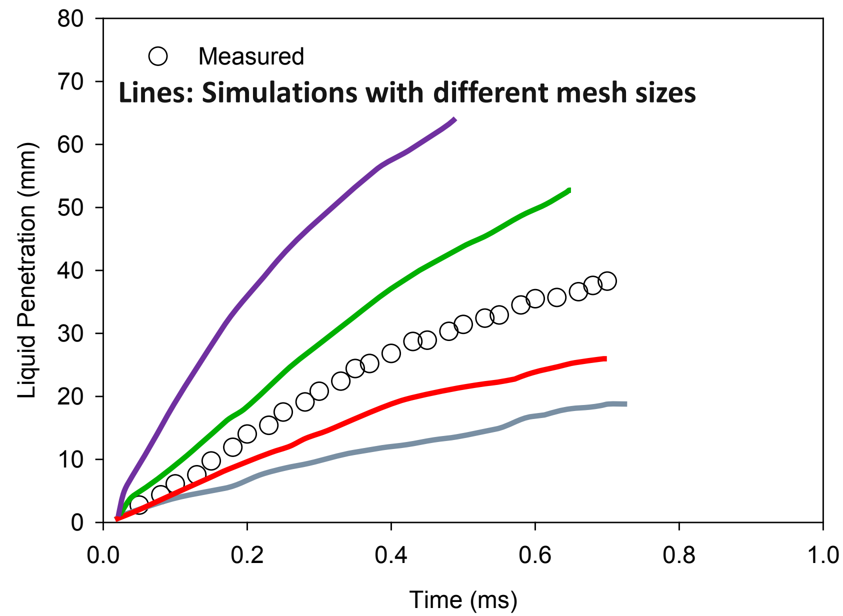
- Nozzle flow and Spray Research
  - Development and validation of in-nozzle flow model against available x-ray radiography data {June 2013}
  - Further validation of LES models against Spray A and Spray H (ECN) data {July 2013}
  - In-nozzle flow simulations with multi-hole diesel injectors {August 2013}
  - Eulerian-Eulerian near nozzle spray model development and validation {September 2013}

- Combustion Modeling with Detailed Chemistry
  - Validating n-dodecane + m-xylene mixture reduced model against experimental data available from Sandia {June 2013}

- High-Performance Computing
  - Further improving scalability of CONVERGE code for engine simulations on up to 2000 processors {September 2013}
  - Using HPC tools for multi-cylinder simulations to capture cylinder to cylinder variations {September 2013}

Approach to Achieving Grid Convergence

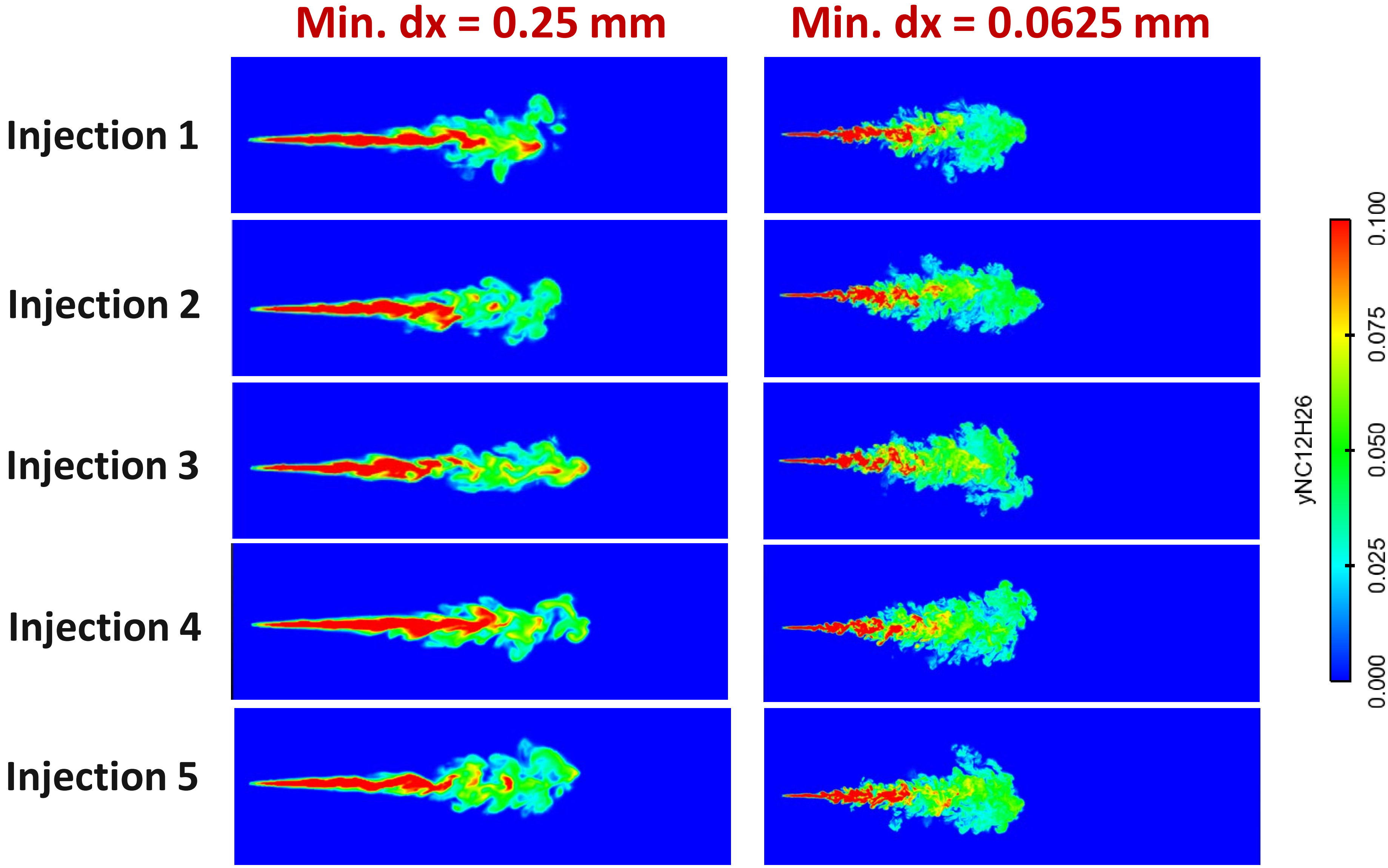
- **Many researchers have reported a strong dependency of the spray on grid size**
- **Adaptive Mesh Refinement (AMR)**
  - Must be able to run cell sizes below the point of convergence
  - Allows the use of very fine grids near the spray while keeping the overall cell count low
- **Fully Implicit Momentum Coupling**
  - Previous studies suffered from instabilities when cell size was on the order of nozzle diameter or smaller



- **Improved Liquid-Gas Coupling**
  - Taylor series expansion to calculate the gas-phase velocity
- **Temporal Liquid Mass Distribution**
  - Significantly increases the injected number of parcels as the grid embedding is increased
- **Spatial Liquid Mass Distribution**

Approach

Cycle-to-Cycle Variations: Dynamic Structure LES



Each injection is perturbed by the different random number seeds to mimic cycle-to-cycle variations in experiments

Approach

Detailed Chemical Mechanisms in Engine Simulations

Typical LLNL mechanism
~1000 species, ~10,000 reactions
Ideal for 0D, 1D simulations

Mechanism Reduction →

Reduced mechanism
~150 species, ~800 reactions
Ideal for 3D-CFD simulations

Computational times scales with $N^2 \sim N^3$

Our Approach:

- Provide the mechanism reductionists with fuel surrogates of interest for the transportation sector
- Extensive validation against ECN spray-combustion and engine data
- Provide feedback on the performance of the reduced mechanism to the mechanism developers, based on 3D-CFD simulations

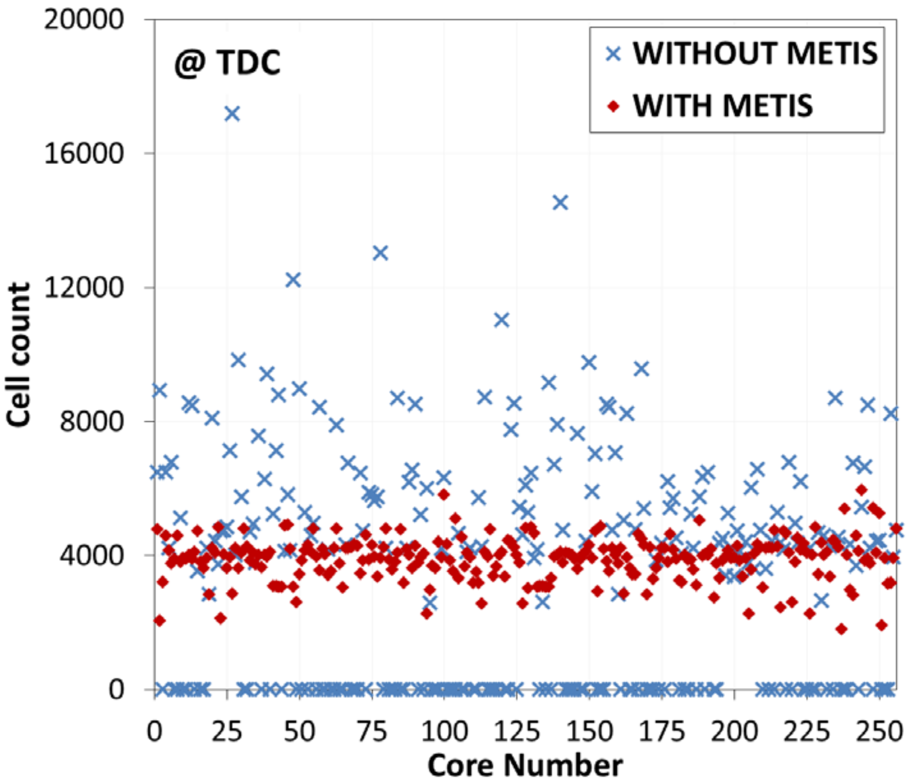
n-Dodecane + m-xylene Mechanism (from LLNL)
2885 species, 11754 reactions

Mechanism Reduction →

Reduced Mechanism
163 species, 887 reactions

Approach

Approach to High-Performance Computing



- METIS is a load-balancing algorithm originally developed at University of Minnesota which has enabled the use of HPC resources
- Significant improvement in load-balancing in CONVERGE due to METIS
- @ TDC the maximum number of CFD cells on a single processor without METIS is 22136, whereas the minimum value is 0. The corresponding values with METIS are 5953 and 1805 respectively

Approach

Diesel Engine Simulations @ Industrial Size Clusters

Typical engine simulation in industry done on 24-64 processors

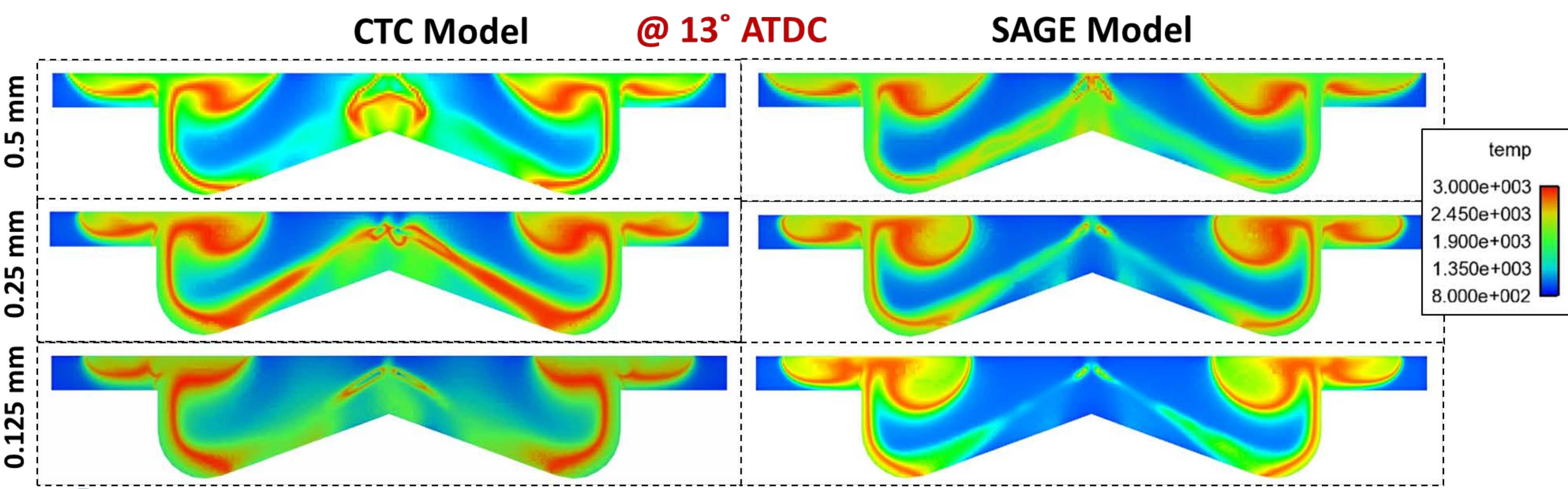
Minimum cell size →	0.5 mm	0.25 mm	0.125 mm
Number of Cores	64	64	256
Peak cell count (in millions)	2.52	8.85	33.69
Wall-clock time (hours:minutes:seconds)	14:06:00	87:56:00	312:33:00
Wall-clock time/computational cycles (s)	7.23	22.42	35.19
	Product Design	Model developments	"one-of-a-kind" simulation

0.125 mm case with ~ 34 million cell count run for ~ 13 days on 256 cores is the **largest diesel engine simulation** performed

Technical Accomplishment and Progress

Simplified vs. Detailed Combustion Models

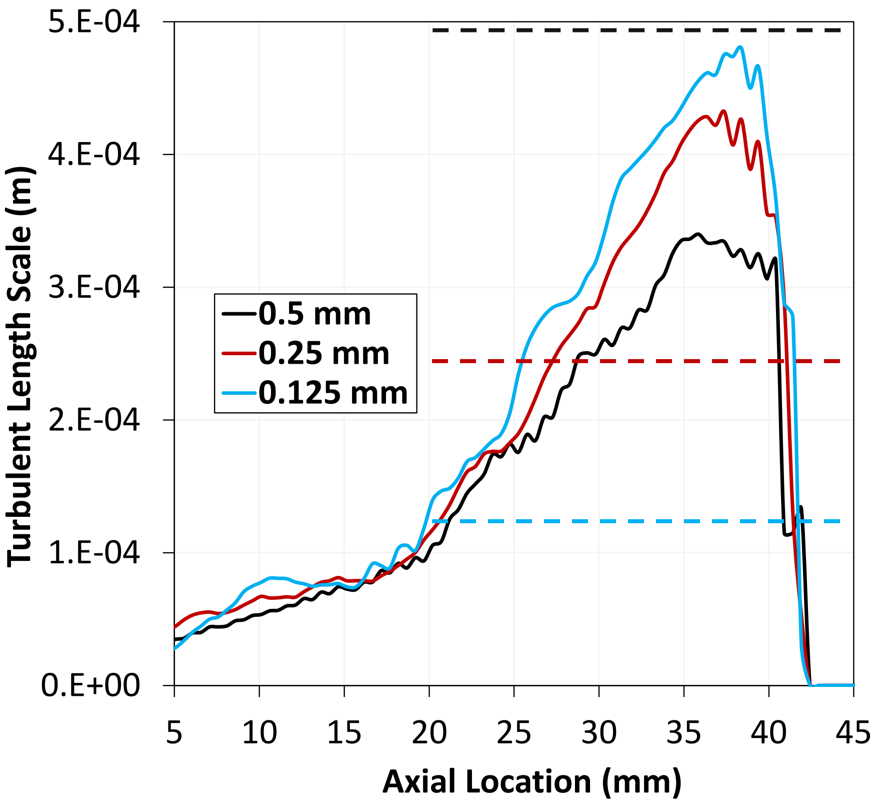
- Caterpillar single-cylinder diesel engine simulated
- Simplified Combustion model: Characteristics time-scale based (CTC) model which incorporates a single global fuel oxidation reaction
- SAGE model is based on detailed chemistry approach
- Simulations with simplified combustion model (CTC model) do not demonstrate grid-convergence
- Simulations with detailed chemistry approach demonstrate grid-convergence on many engine parameters such as pressure, heat release rate, combustion phasing, peak temperatures, etc.

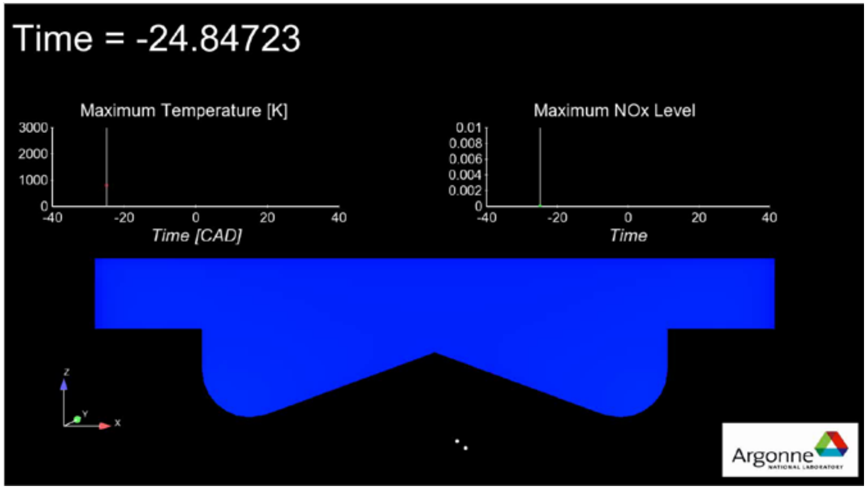


Technical Accomplishment and Progress

How we Achieve Grid-Convergence?

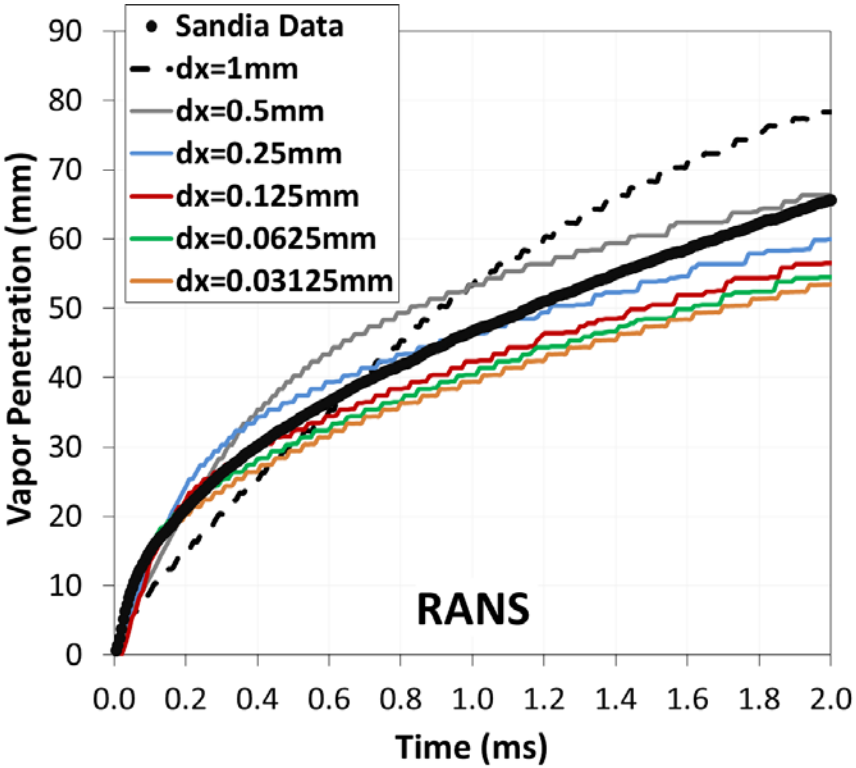
- Turbulent length scales:
  - On the coarse grids (0.5 mm) are lower than the cell sizes hence not resolved
  - On finest grid (0.125 mm) are higher than the cell sizes hence can be resolved
- Turbulent time-scales are grid-convergent at 0.25 mm

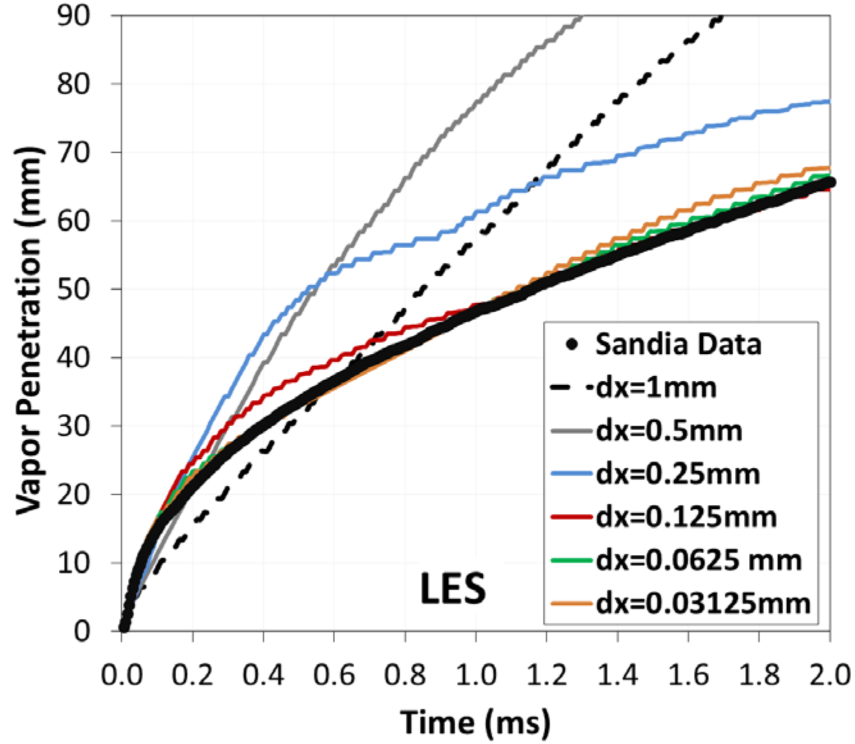




Technical Accomplishment and Progress

Fuel Vapor Penetration: RANS vs. LES

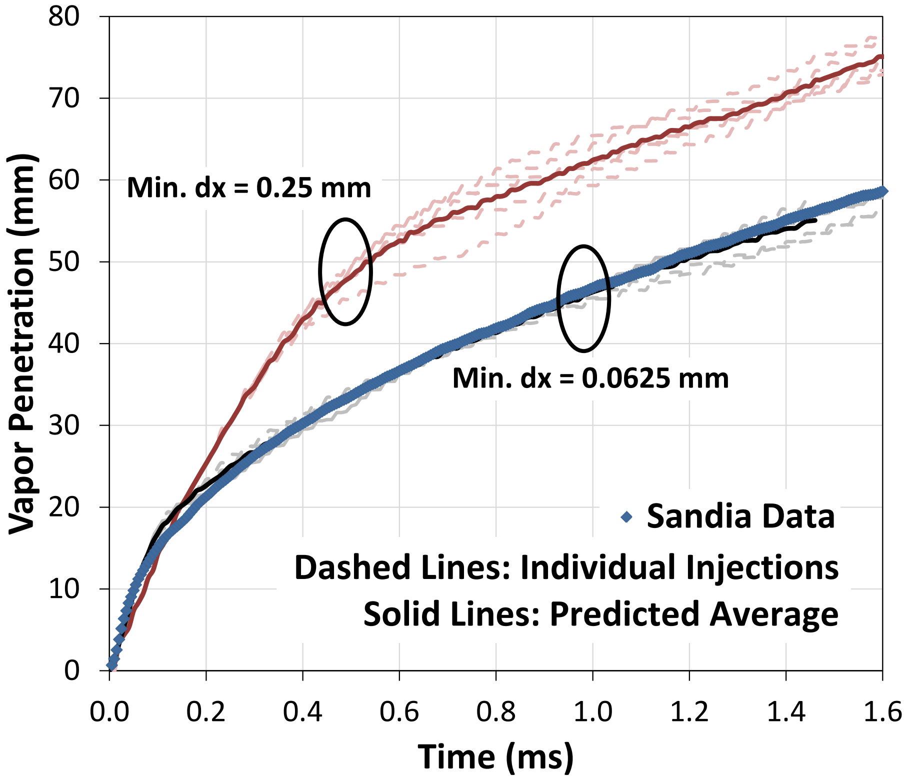


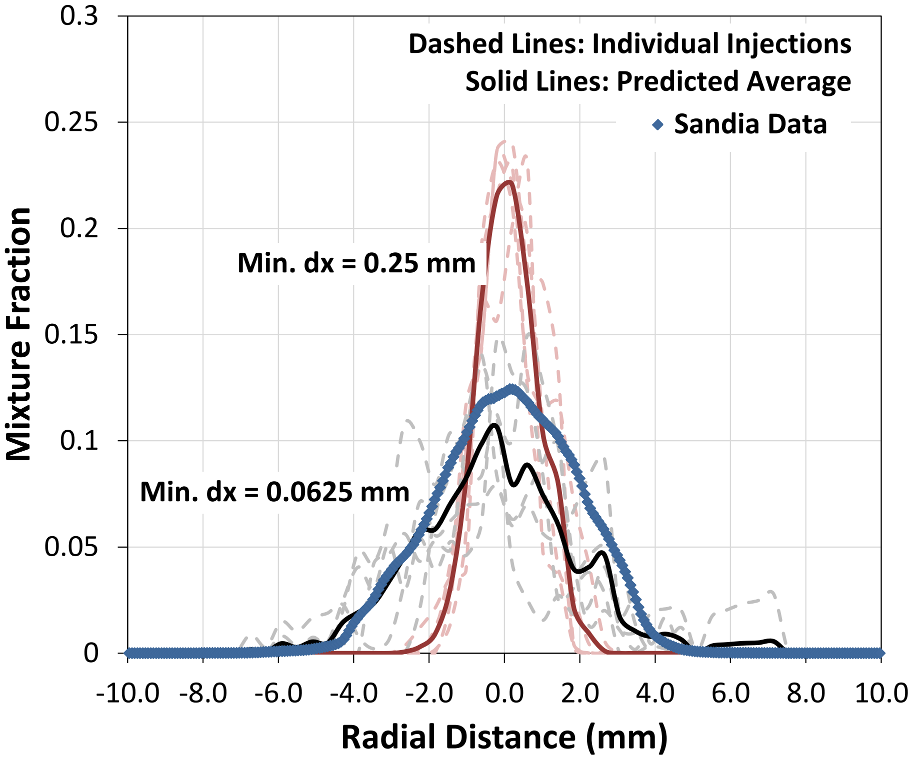


- RANS results though grid-convergent cannot capture the experimental data well
- LES (Dynamic structure model) results are not only grid-convergent but also can capture the experimental data well
- This is due to the fact that LES resolves more flow structures and hence can predict the fuel-air mixing better
- Experimental data for Spray A from Sandia National Laboratory through ECN

Technical Accomplishment and Progress

Cycle-to-Cycle Variations

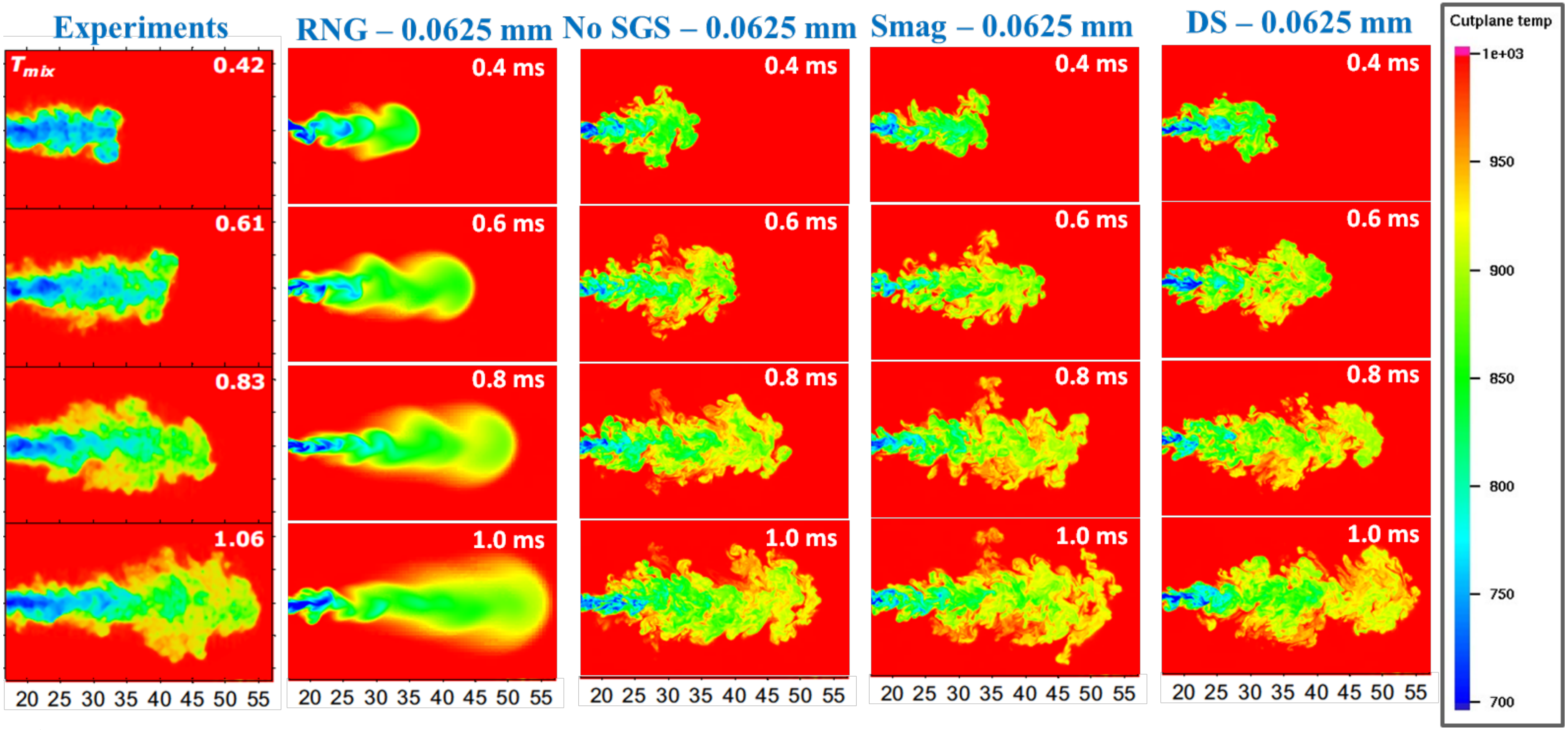




- Global characteristics (spray and vapor penetration) are well represented by a single LES injection event
- Other characteristics (such as mixture fraction, axial velocity distribution) can be captured only by averaging over several LES injections
- Enhancing the resolution improves the predictions for LES
- Averaging over more injections is necessary to further improve finer details such as mixture fraction distribution

Technical Accomplishment and Progress

RANS and LES Approaches



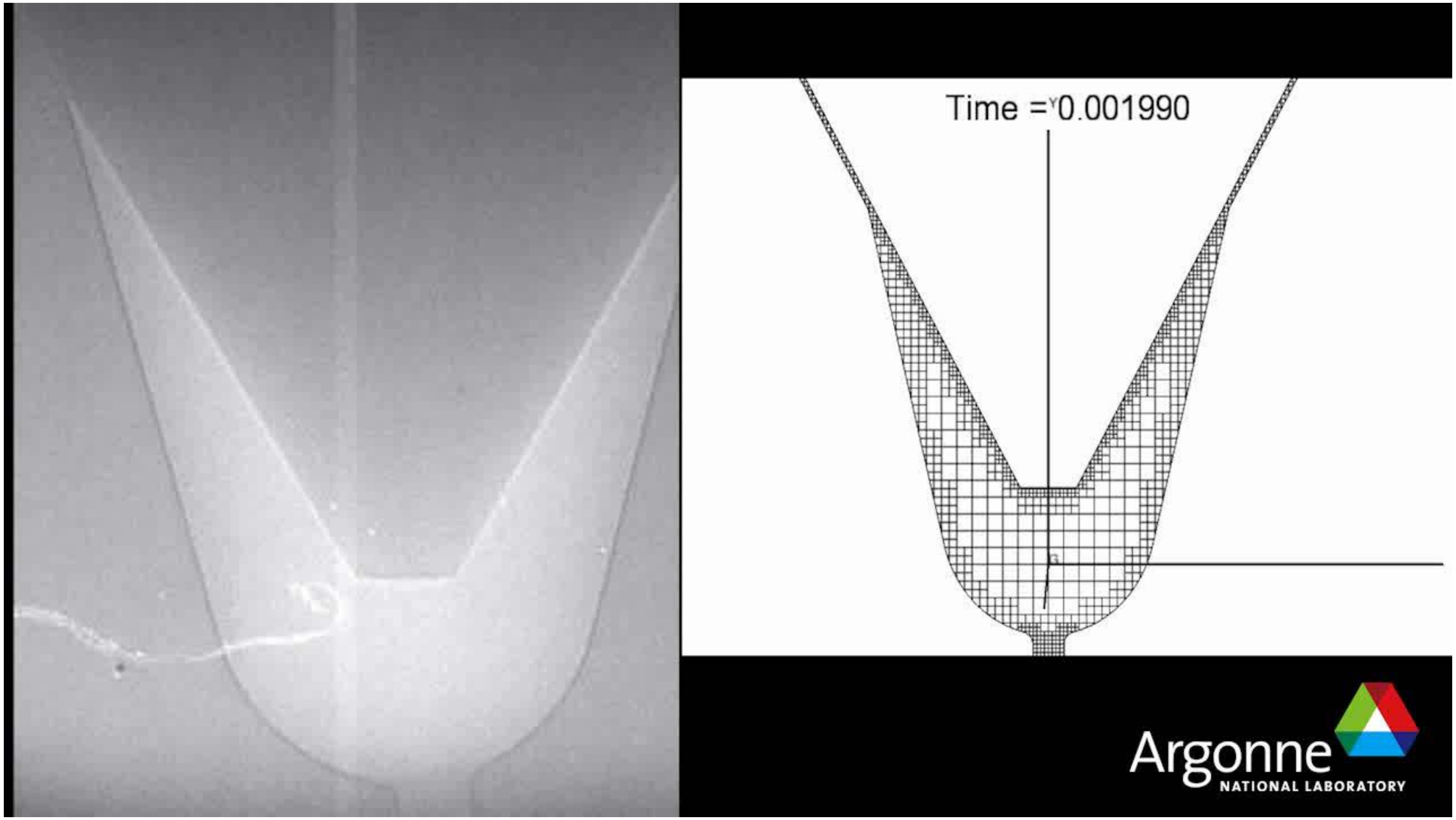
- **Fuel vapor contours represented by gas temperatures are shown**
- All LES models can capture flow structures and qualitatively look similar to the data
- LES results were grid-convergent at 0.0625 mm resolution
- **The computational cost of grid-convergent LES (@0.0625 mm) is about four times compared to grid-convergent RANS (@ 0.25 mm)**

* Experimental data from Pickett et al. SAE Paper No. 2007-01-0647

Technical Accomplishment and Progress

In-Nozzle Simulations using X-ray data

X-ray Phase-Contrast Imaging* | **CFD Simulation**



- Needle lift and **off-axis motion** imposed as a boundary condition
- Able to account for needle off-axis motion effects on nozzle-flow development
- Spray A nozzle from ECN simulated (d_0 = 89 µm)
- Needle lift profile obtained from Dr. Chris Powell at Argonne

Technical Accomplishment and Progress

Diesel Surrogate Mechanism development

Detailed Mechanism (from LLNL)
2885 species, 11754 reactions

↓

DRG – X

↓

DRGASA

↓

Isomer Lumping

↓

DRG – X

↓

DRGASA

↓

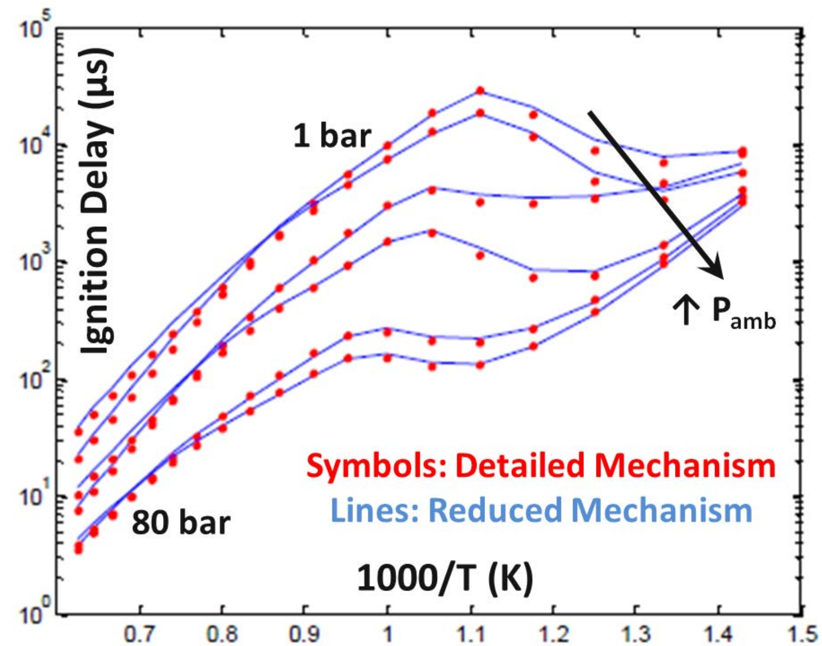
Skeletal Mechanism
163 species, 887 reactions

~ 18 times reduction

DRG related algorithms developed by Prof. T. Lu at University of Connecticut

- n-dodecane (77%) + m-xylene (23%) used as a surrogate for diesel fuel
- Mixture properties recently obtained from NIST

Future Work: Validation against constant volume combustion data from Sandia and engine data at Argonne



Range of operation:
- ✓ Pressure: 1-100 atm
- ✓ Equivalence ratio: 0.5-2.0
- ✓ Initial temperature: 700 – 1800 K

Technical Accomplishment and Progress

Collaborations

Argonne National Laboratory

Engine and Emissions Group: (Provide data for model validation)
Chemical Science and Engineering Group: (Mechanism development and reduction)
Leadership Computing Facility (Improving Scalability of CONVERGE, HPC resources)
Mathematics and Computing Science: (HPC resources)

Convergent Science Inc. (Algorithm and code development in CONVERGE)

Cummins (Provide experimental data, alpha testing of new models)

Caterpillar Inc. (Testing and implementation of HPC tools)

Chrysler LLC. (Dual-Fuel engine data)

Sandia National Laboratory (Provide experimental data through the ECN)

Lawrence Livermore National Laboratory (Mechanism development)

University of Connecticut (Mechanism Reduction)

University of Perugia (Visiting Scholar: Cavitation and Spray Modeling)

Politecnico di Milano (Spray and Combustion modeling using OpenFOAM)

Collaborations and Coordination

ECN Modeling Coordination

University of Wisconsin (USA)

Sandia National Laboratory (USA)

Argonne National Laboratory (USA)

Cambridge University (UK)

Objectives

1) Standardization of spray and combustion parameter definitions
2) Development of engine models
3) Assessing capabilities of different open source and commercial engine modeling codes

CMT (Spain)

Politecnico di Milano (Italy)

TU – Eindhoven (Netherland)

IFP (France)

Georgia Institute of Technology (USA)

UNSW (Australia)

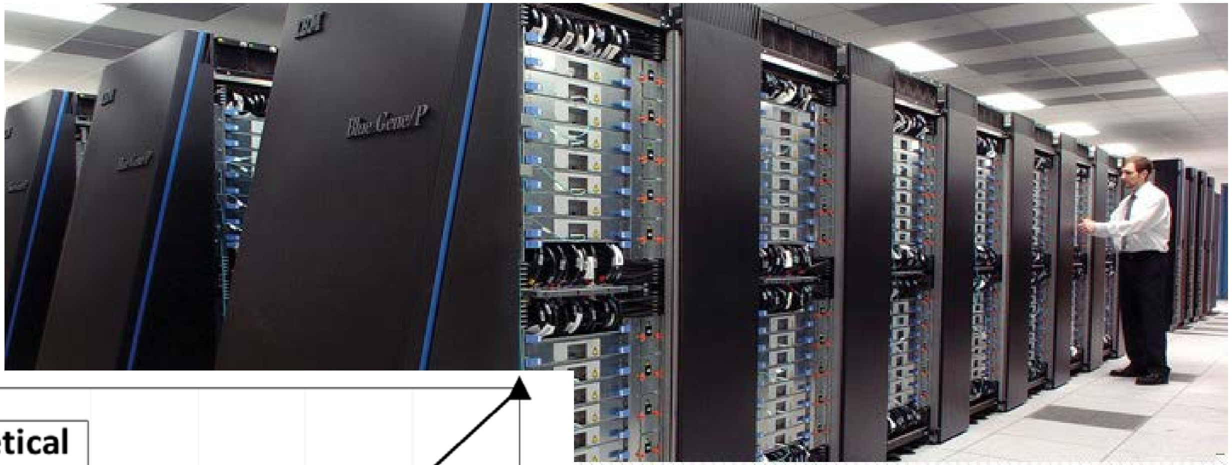
Penn. State (USA)

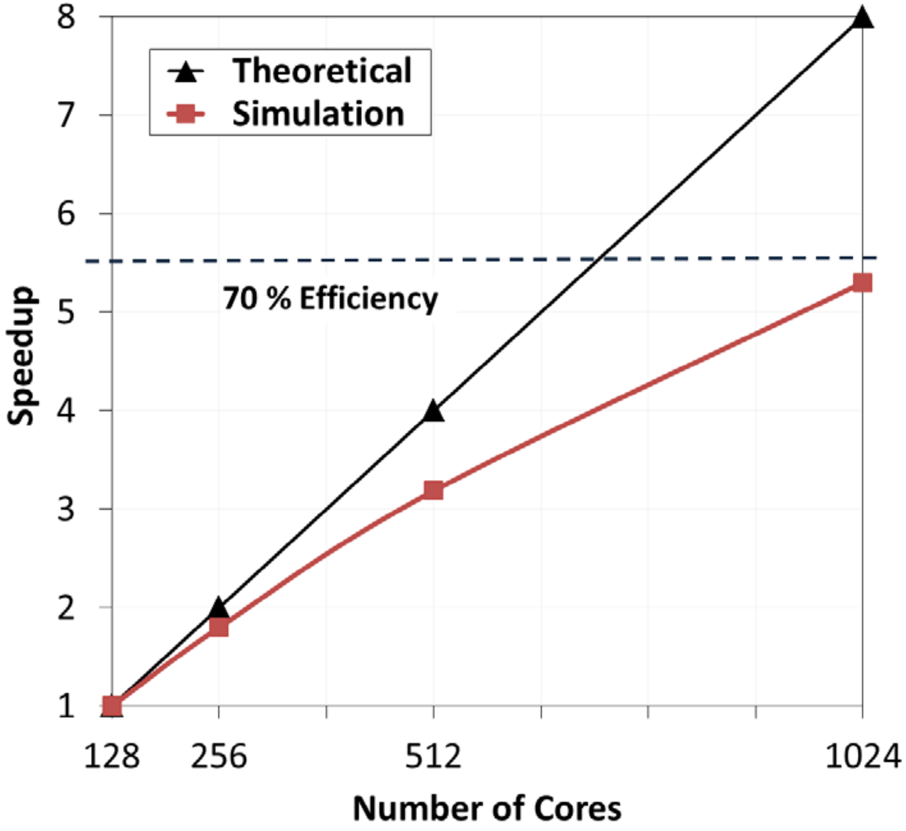
Purdue University (USA)

- Coordinated “Spray development and Vaporization” session in ECN 2 (Heidelberg, September 2012)

Collaborations and Coordination

Future Work using HPC tools





Engine Simulations @ Blue Gene Machine

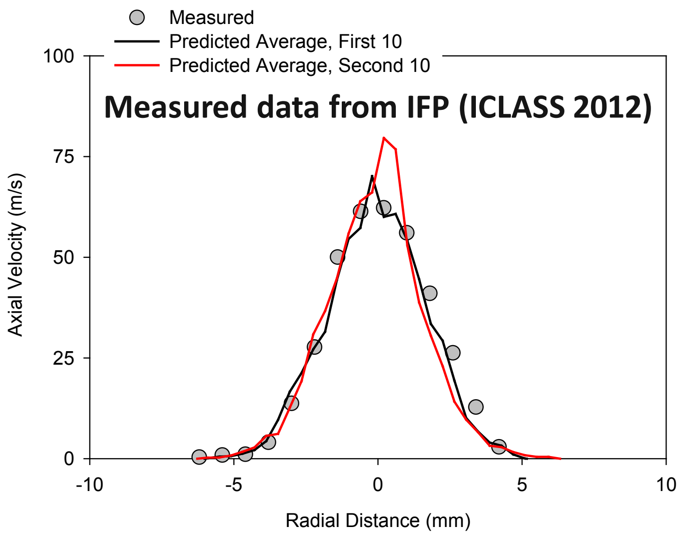
- ✓ CONVERGE compiled for BG architecture
- ✓ Simulation with 13.5 million cells with a minimum grid size of about 150 microns
- ✓ Simulations run in a scalable fashion on 1024 processors

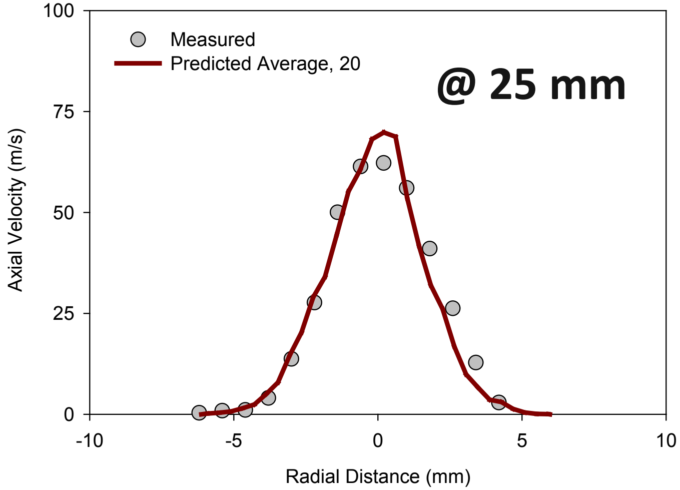
1) **Further enhance scalability by improving I/O issues**
2) **Use HPC to perform high-fidelity multi-cylinder open-cycle simulations**

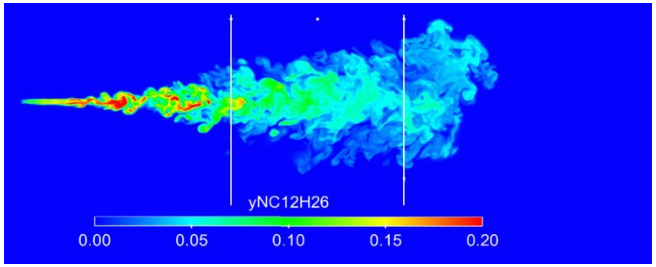
Future Work

CRADA related Future Work

1) In-nozzle flow simulations with Cummins specific hardware
   – X-ray phase contrast imaging in-progress to obtain relevant boundary conditions
2) Eulerian-Eulerian near nozzle flow model
   – Transition to Eulerian-Lagrangian model few nozzle diameters downstream
3) Further validation of the LES models against Spray A and Spray H data from ECN
   – Global parameters (liquid and vapor penetration)
   – Local parameters (axial and radial velocities, mixture fraction distribution etc.)
4) Determine how many LES injections are necessary to mimic all experimental characteristics
   – Already performed 20 injections for Spray A
5) Robust comparison of RANS and different LES models for global and local characteristics together with wall-clock times







Future Work

Quantify the Effect of Needle Motion on Multi-hole Nozzles

- Needle lift-profile was available from Payri et al. (SAE Paper No. 2004-01-2010)
- GM (Mini-sac) nozzle: d_0 = 130 µm; K-factor = 1.5; Hole Length = 1 mm

Future Work

Summary

- **Objective**
  - Development of predictive spray, turbulence, and combustion models aided by high-performance computing tools and comprehensive validation
- **Approach**
  - Coupling expertise from DOE Office of Science on fundamental chemical kinetics, industrial partners, and HPC resources for development of robust engine models
- **Technical Accomplishment**
  - Implemented *improved load balancing* algorithm in CONVERGE which enabled scalable simulations up to 1000 processors using HPC tools
  - Demonstrated *grid-convergent* spray and engine simulations
  - *Cycle-to-Cycle* variations can be captured by a grid-convergent LES approach
  - Effect of *needle off-axis motion* quantified with in-nozzle simulations
- **Collaborations and coordination**
  - with industry, academia, and national laboratories in US
  - through ECN with researchers world-wide
- **Future Work - FY14**
  - Eulerian-Eulerian approach for near nozzle spray modeling
  - Development and validation of realistic diesel surrogate chemical kinetic model
  - Capture cylinder-to-cylinder variations using HPC resources

Technical Back-Up Slides

(Note: please include this "separator" slide if you are including back-up technical slides (maximum of five). These back-up technical slides will be available for your presentation and will be included in the DVD and Web PDF files released to the public.)

3D Spray-Combustion Modeling Set-up

Modeling Tool	CONVERGE Source code access for spray modeling
Dimensionality and type of grid	3D, structured with Adaptive Mesh Resolution
Spatial discretization approach	2nd order finite volume
Smallest and largest characteristic grid size(s)	Base grid size: 1 or 2 mm Finest grid size: 0.03125 mm for Spray simulations Gradient based AMR on the velocity and temperature fields Fixed embedding in the near nozzle region
Total grid number	34 millions is the highest cell count run
Parallelizability	Good scalability on up to 1000 processors

Turbulence model(s)	RANS: RNG k-ε; LES: Smagorinsky, Dynamic Structure, No SGS
Spray models	Breakup: KH-RT without breakup length concept Collision model: NTC, O'Rourke Coalescence model: Post Collision outcomes Drag-law: Dynamic model
In-nozzle Flow	Homogeneous Relaxation Model (HRM)
Time step	Variable based on spray, evaporation, combustion processes
Turbulence-chemistry interactions model	Direct Integration of detailed chemistry well-mixed (no sub-grid model)
Time discretization scheme	PISO (Pressure Implicit with Splitting of Operators)

*** Senecal et al., SAE 2007-01-0159; Som ,PhD. Thesis 2009**

Back-up

Turbulence Models

- Momentum equation

$$\frac{\partial \bar{\rho}\tilde{u}_i}{\partial t} + \frac{\partial \bar{\rho}\tilde{u}_i\tilde{u}_j}{\partial x_j} = -\frac{\partial \bar{p}}{\partial x_i} + \frac{\partial \bar{\sigma}_{ij}}{\partial x_j} - \frac{\partial \tau_{ij}}{\partial x_j}$$

- RANS: RNG k-ε

$$\begin{aligned} \tau_{ij} &= \mu_t \bar{S}_{ij} - \frac{2}{3}\bar{\rho}k\delta_{ij} \\ \mu_t &= \bar{\rho}C_\mu \frac{k^2}{\epsilon} \end{aligned}$$

- LES: Smagorinsky (Smag)
  (Two model constants)

$$\begin{aligned} \tau_{ij} &= -2\bar{\rho}\nu_{sgs}\left(\tilde{S}_{ij} - \frac{1}{3}\delta_{ij}\tilde{S}_{kk}\right) \\ \nu_{sgs} &= C_s^2\Delta^2|\tilde{S}| \end{aligned}$$

- LES: Dynamic structure (DS)
  (No model constants)

$$\begin{aligned} \tau_{ij} &= 2\bar{\rho}k\frac{L_{ij}}{L_{kk}} \\ L_{ij} &= \widehat{\tilde{u}_i\tilde{u}_j} - \hat{\tilde{u}}_i\hat{\tilde{u}}_j \end{aligned}$$

- LES: No SGS - Sub-grid scale turbulence is not modeled but it dissipates

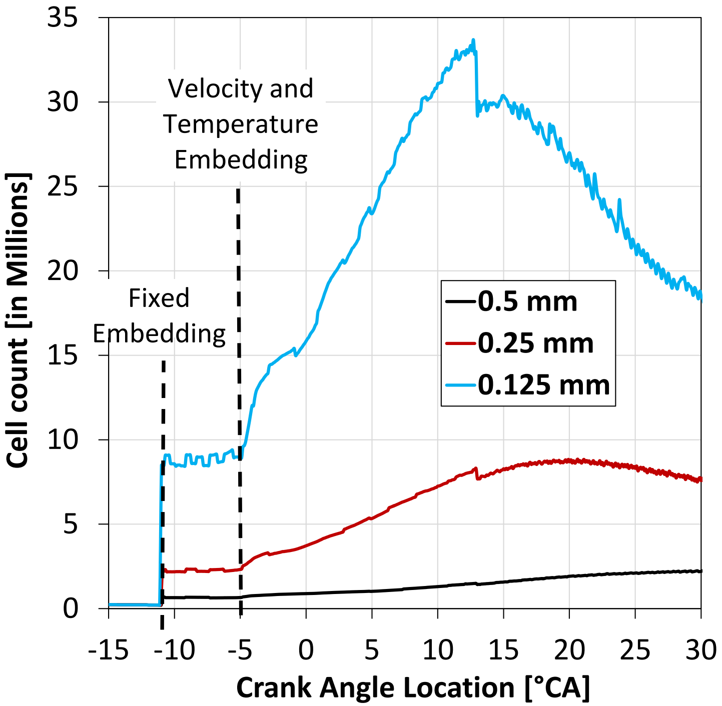
Back-up

CAT Single Cylinder Engine Simulated

Geometry/Parameter	Unit	Value
Fuel		Diesel
Bore	mm	137.16
Stroke	mm	165.1
Compression ratio	-	16:1
Connecting Rod Length	mm	263
Engine speed	rpm	1600
Start of injection	CA˚	-9
Duration of injection	CA˚	21
IVC	CA˚	-147
EVO	CA˚	135
Total fuel mass injected	mg	162.1
Rate of injection	-	Square profile
Fuel Temperature	K	341
Number of orifices	-	6
Nozzle Diameter (d_n)	µm	259

Closed-cycle, full 360˚ engine simulations

Cell count vs. Crank Angle

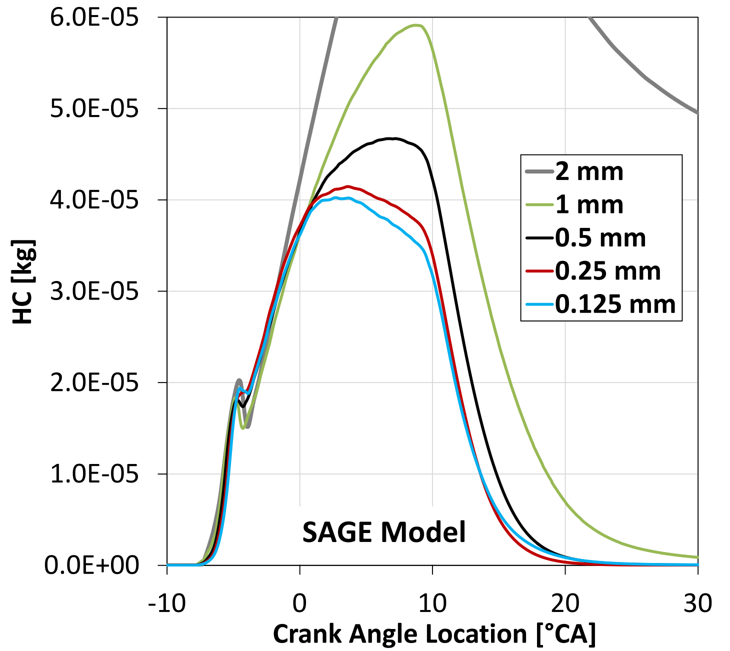


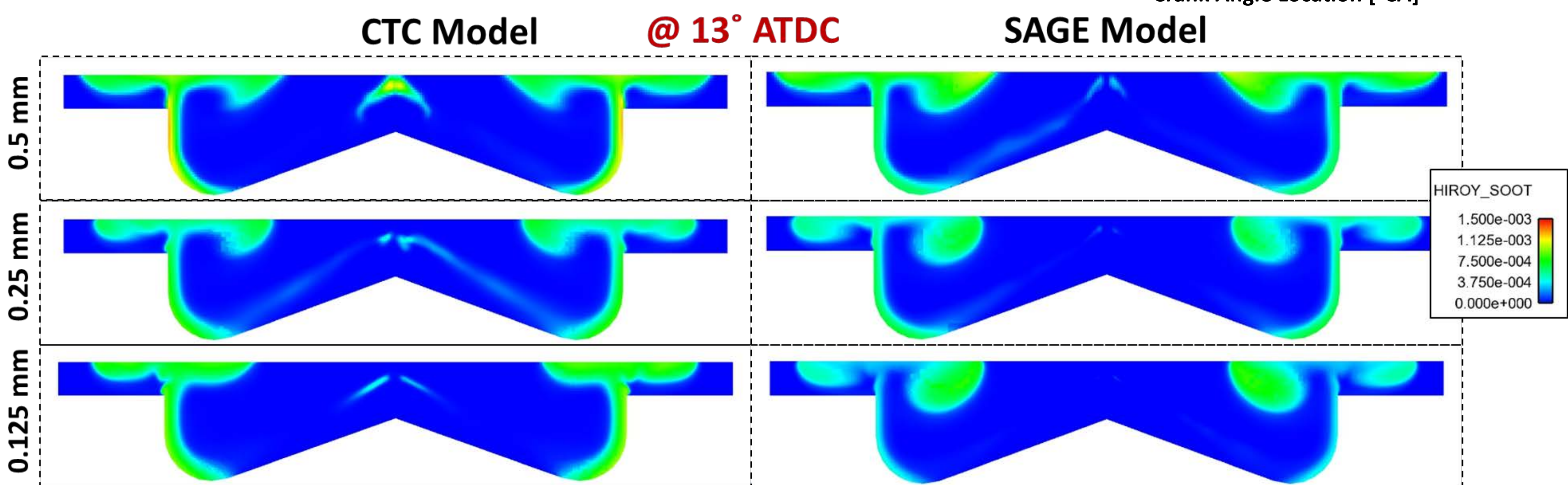
- n-heptane used as a surrogate for diesel fuel (42 species, 168 reaction mechanism from Chalmers University)

Back-up

Simplified vs. Detailed Models: Emission results

- Results with SAGE model are grid-convergent for soot, HC, and CO emissions
- It is not surprising that CTC results are not convergent for emission predictions also
- For emission predictions also a minimum grid size of 0.25 mm is reasonable
- NOx predictions were not grid-convergent and we are looking into this aspect further





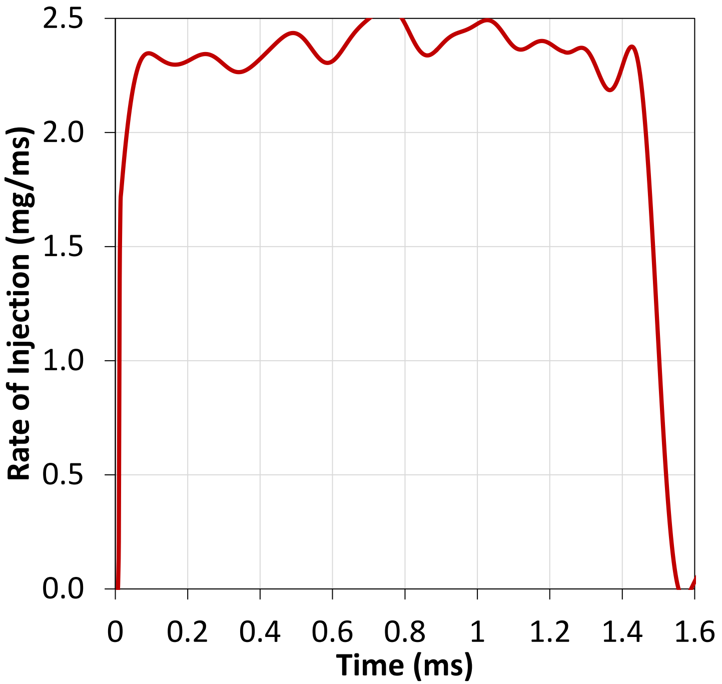
Back-up

Experimental Conditions from ECN

Parameter	Quantity
Fuel	n-dodecane
Nozzle outlet diameter	90 µm
Nozzle K-factor	1.5
Nozzle shaping	Hydro-eroded
Discharge coefficient	0.86
Fuel injection pressure	150 MPa
Fuel temperature	363 K
Injection duration	1.5 ms
Injected fuel mass	3.5 mg
Injection rate shape	Square
Ambient temperature	800 - 1200 K
Ambient gas density	22.8 Kg/m^3
Ambient O_2 Concentration	15 %

http://www.sandia.gov/ecn/

- Experiments performed under both evaporating and combusting conditions.
- Data available for : Spray penetration, liquid length, vapor penetration, mixture fraction, ignition delay, flame lift-off length, soot distribution , high-speed movies



Back-up